Butyl 2-hydroxy-2-methylpropanoate 816-50-2 | DTXSID50278111

Model Performance

Model	Data	
IVIOGEI	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.38

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone

Measured: 1.82 Predicted: 2.23

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2,2-Bis(bromomethyl)-1,3-

propanediol

Measured: 4.79 Predicted: 3.35

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00 Predicted: 1.47

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Paraldehyde Measured: 3.02 Predicted: 2.77

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Bromacil

Measured: 3.24 Predicted: 2.87